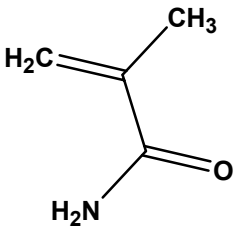
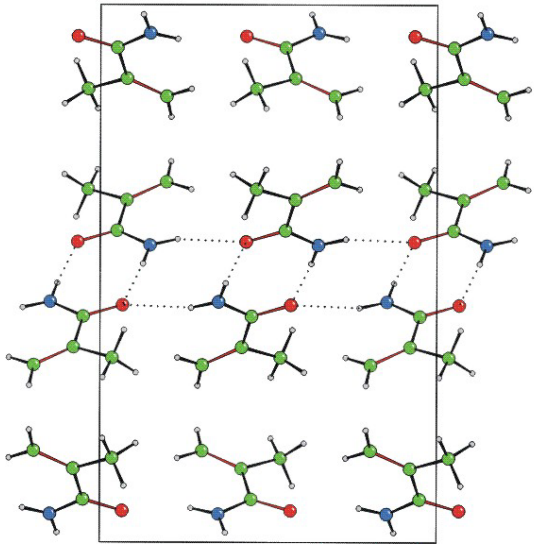
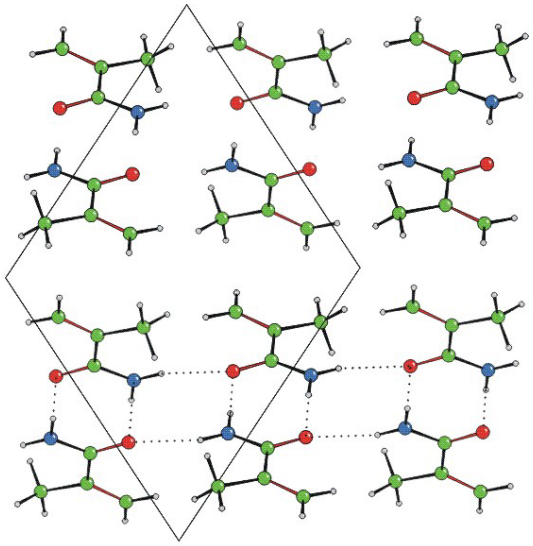
Solid-State Reactions of Molecular Crystals
Bruce M. Foxman, Brandeis University, DMR-0089257

orthorhombic

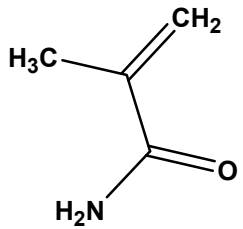


s-trans





monoclinic



s-cis

Polymorphic forms of a crystalline compound have different physical and chemical properties. The industrially important compound methacrylamide was first synthesized in 1928. From 1936 to date, methacrylamide has appeared in over 1000 patents. Methacrylamide sulfate is a key intermediate compound in the ACH process for the manufacture of methyl methacrylate (MMA); the total predicted US capacity for MMA production by the ACH process in 2004 was 1,760 million pounds. As part of a project to study the solid-state reactivity of methacrylamide, graduate student Chengyun Guo grew crystals of methacrylamide and determined their structures by X-ray diffraction. She discovered that there were two conformational polymorphs of methacrylamide, and that their molecular structures correspond to the *s-trans* and *s-cis* conformers; the pair have very similar crystal structures. The two forms have different melting points and physical properties, but their X-ray powder patterns are nearly identical.

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Education & Outreach: Knowledge of space groups and the implications of space group symmetry on the physical and chemical properties of solids are pivotal factors in all areas of structural science. Together with Prof. Jerry Jasinski, whose visit was sponsored as part of the NSF Summer Research Program in Solid-State Chemistry (DMR-0303450), we developed an interactive tutorial of >100 PowerPoint "slides", in four modules, for teaching space groups at the undergraduate and graduate levels. The tutorial, completed in August 2004, has already been adopted for use at the ACS 2004 Summer School in Crystallography (UCSD), University of Oxford (UK) and many other colleges/companies. Discussions are underway with local high school teachers about how we might produce a different version to teach various concepts in symmetry at the secondary school level.

Tutorial features include: diagrams in International Tables (ITX) format, triclinic and monoclinic groups (15) built from "scratch", space groups built iteratively & interactively from ITX symbol, (x,y,z) coordinates that "pop up" as the unit cell is filled, deduction of when and where new symmetry elements appear by visual recognition techniques, links to learned professional societies and important historical figures, and elements of guidance, inquiry and humor to make the learning process enjoyable. The tutorial is packaged as a PowerPoint presentation in a "living book" format. Copies are available for download from http://www.xray.chem.brandeis.edu.

Click & repeat to see Space Group $P\bar{1}$ develop